Connecting via Winsock to STN

Welcome to STN International! Enter x:x

FILE 'HOME' ENTERED AT 11:03:30 ON 18 DEC 2007

=> file reg

Uploading C:\Program Files\Stnexp\Queries\10530986.str

chain nodes :

11 12 13 14 16 18 19 20

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-11 2-12 3-19 7-20 9-14 10-18 11-16 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10

```
10/530986
```

exact/norm bonds :

1-11 9-14 10-18 11-16 12-13

exact bonds : 2-12 3-19 7-20 normalized bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10

G1:H,Ak

G2:H,X

Match level :

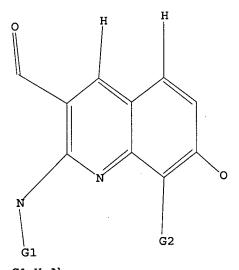
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 16:CLASS 18:CLASS 19:CLASS 20:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 H,Ak G2 H,X

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

L3 208 SEA SSS FUL L1

=> file ca

=> s 13

L4 23 L3

=> d ibib abs fhitstr 1-23

Page 2

ANSWER 1 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:222463 CA

TITLE: Compounds that inhibit HIV particle formation and Rev

protein-dependent HIV production and screening methods

INVENTOR(S): Rekosh, David; Hammarskjold, Marie-Louis

PATENT ASSIGNEE(S): University of Virginia Patent Foundation, USA

SOURCE: PCT Int. Appl., 73 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

| PATENT N | ю. | KI | 4D I | DATE | I | APPLI | CATION | NO. | | DA | TE | |
|---------------------------|-------------------------------|------------------|------------|--------------------|------------|-------|-------------------------------|------------|------------|------------|--------------|-----------|
| WO 20050 | 76861 | A: | 2 2 | 20050825 | V | VO 20 | 05-US3: | .65 | | 20 | 0502 | 201 |
| W: | AE, AG, CN, CO, | CR, CU | CZ, | DE, DK, | DM, | DZ, | EC, EE | EG, | ES, | FI, | GB, | GD, |
| | GE, GH, LK, LR, NO, NZ, | LS, LT | LU, | LV, MA, | MD, | MG, I | MK, MN | MW, | MX, | MZ, | NΑ, | NI, |
| RW: | TJ, TM, BW, GH, | TN, TR GM, KE | TT, LS, | TZ, UA, MW, MZ, | UG, NA, | US, I | UZ, VC SL, SZ | VN, TZ, | YU, UG, | ZA, ZM, | ZM, ZW, | ZW AM, |
| | AZ, BY, EE, ES, RO, SE, | FI, FR | GB, | GR, HU, | IE, | IS, | IT, LT | LU, | MC, | NL, | PL, | PT, |
| | MR, NE, | SN, TD | , TG | | | | | | GIV, | | | |
| CA 25551 PRIORITY APPL | | | L 2 | 20050825 | τ | JS 20 | 05-255! 04-541 | 32P | F | 20 | 0502 | 204 |
| | | | | | τ | JS 20 | 04-569: 04-574: 04-583: | 909P | F F | 20 | 0405 0405 | 527 |
| | | | | | | | 04-363 05-US3 | | _ | | 0502 | |

The present invention describes novel methods of identifying compds. which inhibit HIV particle formation and Rev-dependent HIV production The present invention also provides methods and compds. for inhibiting HIV particle formation and or treating patients infected with HIV. Two cell lines were derived from COS cells to determine anti-Rev activity, Rev-dependent 5BD.1 cells and Rev-independent 2A.22 cells. These cell lines constitutively expressed HIV-like particles that contain the HIV core proteins as well as HIV envelope protein. The non-infectious virions created by these cell are secreted into the media, where a simple p24 ELISA can quant. determine virion production Approx. 40,000 compds. were screened and 192 compds. were identified. The identified compds. were subjected to dose response assays and toxicity assays and 8 compds. were chosen. The eight chosen compds. were tested in a dual luciferase assay for specific inhibition of HIV-1 Rev.

IT 405277-62-5

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(lead compound analog, assay of; compds. that inhibit HIV particle formation and Rev protein-dependent HIV production and screening methods) 405277-62-5 CA

CN 3-Quinolinecarboxamide, 2-amino-6,7-dimethoxy-N-phenyl- (CA INDEX NAME)

RN

Page 5

L4 ANSWER 2 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

141:243319 CA

TITLE:

Polarized ketene dithioacetals as versatile building

blocks for S-containing heterocycles: A new quinoline

synthesis

AUTHOR(S):

Ila, H.

CORPORATE SOURCE:

Dep. Chem., Indian Inst. Technol., Kanpur, 208016,

India

SOURCE:

Kislorod- i Serusoderzhashchie Geterotsikly, [Trudy Mezhdunarodnoi Konferentsii "Khimiya i Biologicheskaya

Aktivnost Kislorod- i Serusoderzhashchikh

Geterotsiklov"], 2nd, Moscow, Russian Federation, Oct.

14-17, 2003 (2003), Volume 1, 246-254. Editor(s): Kartsev, Viktor G. IBS Press: Moscow, Russia.

CODEN: 69EZN9; ISBN: 5-902545-01-3

DOCUMENT TYPE:

Conference

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 141:243319

AB In this lecture, the author has developed a simple, highly efficient and regioselective synthesis of functionalized 2-methylthio-3-substituted quinolines through Vilsmeier cyclization of a variety of α-oxoketene-N,5-acetals. The 2-methylthio functionality in these quinolines has been further manipulated to afford either 2-alkylarylamino quinolines, pyrazolo[3,4-b]quinolines and benzothiopyrano[b]quinolines

through ring annelation with hydrazine hydrate or via radical cyclization.

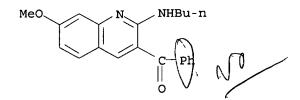
IT 536973-31-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of methylthio-substituted quinolines via Vilsmeier cyclization of α -oxoketene acetals)

RN 536973-31-6 CA

CN Methanone, [2-(butylamino)-7-methoxy-3-quinolinyl]phenyl- (CA INDEX NAME)



REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

140:406718 CA

TITLE:

A facile one-pot synthesis of 2-substituted-3-

aminoquinolines: preparation of benzo[b] naphthyridine-

3-carbonitriles

AUTHOR (S):

Wang, Yanong D.; Boschelli, Diane H.; Johnson, Steven;

Honores, Erick

CORPORATE SOURCE:

Chemical and Screening Sciences, Wyeth Research, Pearl

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

River, NY, 10965, USA

SOURCE:

Tetrahedron (2004), 60(13), 2937-2942

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 140:406718

AB A facile one-pot synthesis of 3-aminoquinolines from orthoaminobenzaldehydes was developed. Et 6,7-dimethoxy-3-aminoquinoline-2carboxylate, a key intermediate for the preparation of a 4-anilinobenzo[b][1,5]-naphthyridine-3-carbonitrile, was efficiently prepared by this method. Synthetic routes to 4-anilino-benzo[b][1,5]-naphthyridine-3carbonitrile and 4-anilino-benzo[b][1,8]-naphthyridine-3-carbonitrile are described.

IT 348618-70-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(one-pot synthesis of 2-substituted-3-aminoquinolines for use as synthons toward the preparation of benzo[b] naphthyridine-3-carbonitriles)

RN 348618-70-2 CA

CN 3-Quinolinecarboxylic acid, 2-amino-6,7-dimethoxy-, methyl ester (CA INDEX NAME)

MeO NH2

C-OMe

REFERENCE COUNT:

9

L4 ANSWER 4 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 140:375083 CA

TITLE: Preparation of quinoline-3-carboxylic acids as YAK3

inhibitors

INVENTOR(S): Burgess, Joelle L.; Callahan, John F.; Hamajima,

Toshihiro; Ida, Satoru; Tang, Jun; Mori, Ichiro

Smithkline Beecham Corporation, USA

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PA' | TENT | NO. | | | KIN |) | DATE | | | APPI | JICAT | ION I | NO / | | D. | ATE | |
|--------------|-------|------|----------|-----|-----|-----|------|------|-----|------|---------|-------|--------|-----|-----|------|-----|
| - - · | | | - | | | - | | | | | | | ード・ナン・ | | - | | |
| WO | 2004 | 0349 | 85 | | A2 | | 2004 | 0429 | | WO 2 | 2003- | US32 | 625 | | 2 | 0031 | 015 |
| WO | 2004 | 0349 | 85 | | A3 | | 2004 | 0910 | | | | | • | | | | |
| | W: | ΑE, | AG, | AL, | AM, | ΑT, | AU, | ΑZ, | BA, | BB, | ВG, | BR, | BY, | ΒZ, | CA, | CH, | CN, |
| | | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, | GE, |
| | | GH, | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KP, | KR, | KZ, | LC, | LK, |
| | | LR. | LS, | LT. | LU, | LV. | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NI, | NO, | NZ, |
| | | • | • | - | | | | | - | | SE, | | | | | | |
| | | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VC, | VN, | YU, | ZA, | ZM, | ZW | | |
| | RW: | GH, | GM, | ΚE, | LS, | MW, | ΜZ, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | AZ, | BY, |
| | | KG, | ΚZ, | MD, | RU, | ТJ, | TM, | ΑT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, |
| | | FI, | FR, | GB, | GR, | HU, | IE, | IT, | LU, | MC, | NL, | PT, | RO, | SE, | SI, | SK, | TR, |
| | | BF, | ВJ, | CF, | CG, | CI, | CM, | GΑ, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, | TG |
| AU | 2003 | | | | | | | | | | | | | | | | |
| EP | 1556 | 379 | | | A2 | | 2005 | 0727 | | EP 2 | 2003- | 7763 | 96 | | 2 | 0031 | 015 |
| | | | | | | | | | | | IT, | | | | | | |
| | | | | | | | | | | | TR, | | | | | | |
| JР | 2006 | 5030 | 94 | | Т | | 2006 | 0126 | | JP 2 | 2004- | 5453 | 0.2 | | 2 | 0031 | 015 |
| US | 2006 | 1060 | 58 | | A1 | | 2006 | 0518 | | US 2 | سر 5005 | 5309 | 86 | | 2 | 0050 | 412 |
| PRIORIT | | | | | | | | | | | 2002 | | | | | | |
| | | | | • | | | | | | | 2003- | | | | | 0031 | |
| OTHER S | OURCE | (S): | | | MAR | PAT | 140: | 3750 | | | | | | | | | |

The title 3-carboxy quinoline derivs. [I; R1 = H, alkyl; R2 = (Q)q(Q1)rQ2 (wherein Q = CH2; q = 0-4; Q1 = O, NH, CH(OH); r = 0-1; Q2 = H, alkyl, aryl, etc.); R3, R3a = H, alkyl, hydroxyalkyl; m, n = 0-1; or m = 1 and n = 1 and R3 and R3a together with the atoms to which they are attached form (un)substituted fused ring II, III; R4 = OH, NHSO2Rc, NRbR; R5 = H, halo; R = H, aryl, ORb; Rb = H, alkyl, alkenyl; Rc = aryl, alkyl] which are useful as YAK3 inhibitors, were prepared Thus, reacting 2-chloro-7-methoxyquinoline-3-carboxylic acid with tert-Bu (3-aminopropyl)carbamate followed by Boc-group removal afforded

GI

CN

2-(3-aminopropylamino)-7-methoxyquinoline-3-carboxylic which showed pIC50 of 6.0 in hYAK3 assay. The invention also includes methods of making the compds. I as well as methods of using the same in the treatment of diseases mediated by inappropriate YAK3 activity. The pharmaceutical composition comprising the compound I is claimed.

IT 683749-55-5P, 2-((3-tert-Butoxycarbonylaminopropyl)amino)-7methoxyquinoline-3-carboxylic acid
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of quinoline-3-carboxylic acids as YAK3 inhibitors)

RN 683749-55-5 CA

3-Quinolinecarboxylic acid, 2-[[3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]amino]-7-methoxy- (CA INDEX NAME)

MeO NH- (CH₂)₃-NH-C-OBu-t
$$CO_{2}H$$

L4 ANSWER 5 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

139:285650 CA

TITLE:

Inhibition of Src kinase activity by

4-anilino-5,10-dihydro-pyrimido[4,5-b]quinolines

AUTHOR(S): Boschelli, Diane H.; Powell, Dennis; Golas, Jennifer

M.; Boschelli, Frank

CORPORATE SOURCE:

Chemical and Screening Sciences, Wyeth Research, Pearl

River, NY, 10965, USA

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2003),

13(18), 2977-2980

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 139:285650

AB 4-(2,4-Dichloro-5-methoxy)anilino-5,10-dihydropyrimido[4,5-b]quinolines are potent inhibitors of Src kinase and Src cellular activity while having no effect on Fyn cellular activity. The corresponding

4-(2,4-dichloro-5-methoxy)anilino-pyrimido[4,5-b]quinolines are much less effective Src inhibitors.

IT 609343-56-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and Src kinase-inhibiting activity of 4-anilino-5,10-dihydro-pyrimido[4,5-b]quinolines)

RN 609343-56-8 CA

CN 3-Quinolinecarboxylic acid, 2-amino-6-methoxy-7-(2-methoxyethoxy)-, methyl ester (CA INDEX NAME)

REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 139:22099 CA

TITLE: Reaction of α -Oxoketene-N,S-arylaminoacetals

with Vilsmeier Reagents: An Efficient Route to Highly Functionalized Quinolines and Their Benzo/Hetero-Fused

Analogues

AUTHOR(S): Mahata, P. K.; Venkatesh, C.; Kumar, U. K. Syam; Ila,

H.; Junjappa, H.

CORPORATE SOURCE: Department of Chemistry, Indian Institute of

Technology, Kanpur, 208016, India

SOURCE: Journal of Organic Chemistry (2003), 68(10), 3966-3975

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE:

OTHER SOURCE(S):

Journal English

LANGUAGE:

CASREACT 139:22099

GI

$$R^{1}$$
 R^{2}
 R^{2}
 R^{2}
 R^{2}
 R^{2}
 R^{2}
 R^{2}
 R^{2}
 R^{3}
 R^{2}
 R^{2}
 R^{3}
 R^{2}
 R^{3}
 R^{2}
 R^{3}
 R^{4}
 R^{2}
 R^{4}
 R^{4

A simple, highly efficient, and regioselective synthesis of functionalized AB quinolines I [R1 = H, 7-MeO, 7-F, 6,7-(MeO)2, etc.; (R2 = Ph, 2-BrC6H4, (MeO)2CH; R3 = H, Me] via Vilsmeier cyclization of a variety of α-oxoketene-N,S-aminoacetals II was reported. The cyclization is facile with N,S-acetals bearing strongly activating groups on aniline aromatic ring, whereas in other cases the yields of quinolines are moderate. The reaction could be extended to the synthesis of substituted tricyclic benzo[h]quinoline, pyrido[2,3-h]quinoline, 4,7-diphenylphenanthroline, and tetracyclic quino[8,7-h]quinoline by performing a Vilsmeier reaction on N, S-acetals derived from 1-naphthylamine, m-phenylenediamine, o-phenylenediamine, and 1,5-diaminonaphthalene, resp. Some quinolines I were subjected to further transformations, such as reduction with Raney-Ni in EtOH, oxidation with N-bromosuccinimide or sequential m-CPBA oxidation/amine substitution, to afford 2-unsubstituted quinolines, quinoline-5,8quinones, or 2-alkyl/aryl aminoquinolines, resp. Similarly, cycloannulation of 2-methylthio-3-benzoylquinolines I (R2 = Ph) with hydrazine hydrate under microwave irradiation afforded the corresponding substituted and fused pyrazolo[3,4-b]quinolines in excellent yields, whereas intramol. radical cyclization of I (R2 = 2-BrC6H4) yielded the corresponding benzothiopyrano-fused quinolines.

IT 536973-31-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of functionalized quinolines and their benzo/hetero-fused analogs via benzannulation of α -oxoketene-N,S-arylaminoacetals with Vilsmeier reagents)

RN 536973-31-6 CA

CN Methanone, [2-(butylamino)-7-methoxy-3-quinolinyl]phenyl- (CA INDEX NAME)

82

THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:338091 CA

TITLE: Synthesis of some novel quinoline-3-carboxylic acids

and pyrimidoquinoline derivatives as potential

antimicrobial agents

AUTHOR(S): El-Sayed, Ola A.; Al-Bassam, Badr A.; Hussein, Maher

E.

CORPORATE SOURCE: Pharmaceutical Chemistry Department, Faculty of

Pharmacy, University of Alexandria, Alexandria, 21215,

Egypt

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2002),

335(9), 403-410

CODEN: ARPMAS; ISSN: 0365-6233 Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:338091

GI

PUBLISHER:

The synthesis and in vitro antimicrobial evaluation of several quinoline AB and pyrimidoquinoline derivs. are described. Treatment of 7-substituted 2-oxo-3-quinolinecarboxylic acids with phosphoryl chloride or thionyl chloride gave rise to the 7-substituted 2-chloro-3-quinolinecarboxylic acids and 7-substituted 2-chloro-3-quinolinecarbonyl chlorides, resp. Reaction of 2-chloro-3-quinolinecarboxylic acids with 2-thiazolamine or 2-pyridinamine gave 2-[(2-thiazolyl)amino]-3-quinolinecarboxylic acids and 2-[(2-pyridinyl)amino]-3-quinolinecarboxylic acid, resp. Treatment of 2-chloro-3-quinolinecarbonyl chlorides the same heterocyclic amines at room temperature furnished the corresponding 2-chloro-N-(2-thiazoly1)-3quinolinecarboxamides I (R = H, Me, OMe) and 2-chloro-N-(2-pyridinyl)-3quinolinecarboxamides II (R = H, Me, OMe). The tetracyclic 9-substituted thiazolo[3',2':1,2]-pyrimido[4,5-b]quinolin-5-ones III (R = H, Me, OMe) and 10-substituted pyrido[1',2':1,2]pyrimido[4,5-b]quinolin-6-ones IV (R = H, Me, OMe) were synthesized by heating 2-chloro-3-quinolinecarbonyl chlorides with the heterocyclic amines in toluene or by heating I or II under reflux in DMF. The products were evaluated in vitro for potential antimicrobial activity.

IT 517917-85-0P, 7-Methoxy-2-[(2-Thiazolyl)amino]-3-

quinolinecarboxylic acid

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of quinolinecarboxylic acids and pyrimidoquinoline derivs. and their activity as antimicrobial agents)

RN 517917-85-0 CA

CN 3-Quinolinecarboxylic acid, 7-methoxy-2-(2-thiazolylamino)- (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:24657 CA

Synthesis of cyclopenta[b]benzo[g][1,8]naphthyridines TITLE:

Prakash, G. Arul; Kumar, N. Sampath; Rajendran, S. P. AUTHOR (S):

Department of Chemistry, Bharathiar University, CORPORATE SOURCE:

Coimbatore, 641 046, India

Asian Journal of Chemistry (2002), 14(3-4), 1303-1306 CODEN: AJCHEW; ISSN: 0970-7077 SOURCE:

PUBLISHER: Asian Journal of Chemistry

Journal DOCUMENT TYPE: English LANGUAGE:

CASREACT 138:24657 OTHER SOURCE(S):

2-Chloro-3-formylquinoline and its derivs. were prepared and aminated by dry AB ammonia gas in ethanol. The 2-amino-3-formylquinolines so obtained were then condensed with cyclopentanone in presence of acetic acid and sulfuric acid to give benzo[g]cyclopenta[b][1,8]naphthyridines.

IT 264135-40-2P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn.of cyclopenta[b]benzo[g][1,8]naphthyridines by condensation of 2-amino-3-formylquinolines with cyclopentanone)

RN 264135-40-2 CA

3-Ouinolinecarboxaldehyde, 2-amino-7-methoxy- (CA INDEX NAME) CN

NH₂ MeO

REFERENCE COUNT THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 23 CA COPYRIGHT 2007 ACS on STN -

ACCESSION NUMBER: 137:310824 CA

TITLE: Preparation of quinoline inhibitors of hYAK1 and hYAK3

kinases

INVENTOR(S): Bryan, Deborah L.; Burgess, Joelle L.; Callahan, James

Smithkline Beecham Corporation, USA PATENT ASSIGNEE(S):

PCT Int. Appl., 53 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT 1 | NO. | KIND I | DATE | APPLICATION NO. | DATE |
|-------------------------------|--|--|--|--|--|
| | 081728 081728 | A2 2 | 20021017 | WO 2002-US10657 | 20020404 |
| W: | CO, CR, CU GM, HR, HU LS, LT, LU PL, PT, RO | CZ, DE, ID, IL, LV, MA, RU, SD, | DK, DM, IN, IS, MD, MG, SE, SG, | BA, BB, BG, BR, BY, BZ DZ, EC, EE, ES, FI, GB JP, KE, KG, KP, KR, KZ MK, MN, MW, MX, MZ, NC SI, SK, SL, TJ, TM, TN | G, GD, GE, GH, LC, LK, LR, NZ, OM, PH, |
| | CY, DE, DK | LS, MW, ES, FI, CG, CI, | MZ, SD, FR, GB, CM, GA, | ZM, ZW SL, SZ, TZ, UG, ZM, ZW GR, IE, IT, LU, MC, NL GN, GQ, GW, ML, MR, NE AU 2002-256085 | PT, SE, TR, SN, TD, TG |
| EP 1372 | 654 | A2 2 | 20040102 | EP 2002-725526 | 20020404 |
| JP 2004 US 2005 US 7087 | IE, SI, LT 526756 043352 758 | LV, FI, T 2 A1 2 | RO, MK, 20040902 20050224 | GB, GR, IT, LI, LU, NL CY, AL, TR JP 2002-580090 US 2003-474084 | 20020404 20031006 |
| PRIORITY APPORTER SOURCE | | MARPAT 1 | 137:31082 | US 2001-282229P WO 2002-US10657 | |

I

GI

The title compds. [I; R6 = NHalkyl, NHcycloalkyl, NHaryl, etc.; R7 = CO2H, AB CONH2, CHNOH, etc.; R8 = H, OH, alkyl, etc.; R9 = H, alkyl, cycloalkyl, etc.; R8 and R9 can form a 5-7 membered ring comprising heteroatoms selected from O, N, and S; R10 = H, halo], useful in the treatment of diseases in which an excessive amount of either hYAK1 and hYAK3 kinases is a factor, were prepared Thus, reacting 2-chloro-7-methoxyquinoline-3carboxylic acid with 3-chloroaniline in xylene afforded I [R6 = 3-ClC6H4NH; R7 = CO2H; R8 = OMe; R9, R10 = H]. The compds. I showed IC50 of 0.01-10 μ M, and 0.03-10 μ M against hYAK1 and hYAK3, resp. IT 470701-99-6P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

Page 16

RN 470701-99-6 CA

CN 3-Quinolinecarboxylic acid, 2-[(3-chlorophenyl)amino]-7-methoxy- (CA INDEX NAME)

CA COPYRIGHT 2007 ACS on STN ANSWER 10 OF 23

ACCESSION NUMBER:

136:37618 CA

TITLE:

Preparation of substituted aromatic tricyclic

compounds containing nicotinonitrile rings as protein

kinase inhibitors

INVENTOR(S):

Berger, Dan M.; Dutia, Minu D.; Demorin, Frenel F.; Boschelli, Diane H.; Powell, Dennis W.; Tsou, Hwei-ru;

Wissner, Allan; Zhang, Nan; Ye, Fei; Wu, Biqi American Home Products Corporation, USA; Wyeth

PATENT ASSIGNEE(S):

U.S. Pat. Appl. Publ., 107 pp.

SOURCE:

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|-----------|-------------------|----------|
| | | | | |
| US 2001051620 | A1 | 20011213 | US 2000-751274 | 20001229 |
| US 6638929 | B2 | 20031028 | | |
| US 2004110762 | A1 | 20040610 | US 2003-618044 | 20030710 |
| US 7105531 | B2 | 20060912 | | |
| US 2006247217 | A1 | 20061102 | US 2006-478121 | 20060629 |
| PRIORITY APPLN. INFO.: | | | US 1999-240905P P | 19991229 |
| | | | US 2000-751274 A3 | 20001229 |
| | | | US 2003-618044 A3 | 20030710 |
| OTHER SOURCE(S): | MARPAT | 136:37618 | | |

OTHER SOURCE(S):

GI

The title compds. I [Ar = (un) substituted cycloalkyl, pyridyl, AΒ pyrimidinyl, etc.; n = 0-1; X = NH, O, S, NR; R = alkyl; Y, Z = both carbon or N; A = (un)substituted benzo, pyrido, pyrimido, etc.] which are useful as inhibitors of protein tyrosine kinase and are antiproliferative agents, were prepared E.g., a 3-step synthesis of II which showed IC50 of 0.005 µM against EGF-R kinase (recombinant enzyme), was given.

348618-70-2P IT

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted aromatic tricyclic compds. containing nicotinonitrile

rings as protein kinase inhibitors)

RN 348618-70-2 CA

3-Quinolinecarboxylic acid, 2-amino-6,7-dimethoxy-, methyl ester (CA CN INDEX NAME)

ANSWER 11 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

135:92639 CA

TITLE:

Preparation of substituted aromatic tricyclic

compounds containing nicotinonitrile rings as protein

kinase inhibitors

INVENTOR(S):

Berger, Dan M.; Dutia, Minu D.; Demorin, Frenel F.; Boschelli, Diane H.; Powell, Dennis W.; Tsou, Hwei-ru;

Wissner, Allan; Zhang, Nan; Ye, Fei; Wu, Biqi

American Home Products Corp., USA

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 377 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PA: | TENT | NO. | | | KINI | D | DATE | | | APF | LICAT | CION | NO. | | | DATE | |
|--------|-------|------|------|-----|------|-----|------|-------|-----|-----|--------|-------|------|-----|------------|-------|-----|
| WO | 2001 | 0478 | 92 | | Al | - | 2001 | 0705 | | WO | 2000- | ·US35 | 616 | | | 20001 | 229 |
| | | | | | | | | | | | BG, | | | | | | |
| | | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EE, | ES | , FI, | GB, | GD, | GE, | GH | , GM, | HR, |
| | | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KF | , KR | KZ, | LC, | LK, | LR | , LS, | LT, |
| | | LU, | LV, | MA, | MD, | MG. | MK, | MN, | MW, | MX | , MZ | NO, | NZ, | PL, | PT | , RO, | RU, |
| | | SD, | SE, | SG, | SI, | SK | SL, | TJ, | TM, | TR | , TT | TZ, | UA, | UG, | UZ | , VN, | YU, |
| | | ZA, | zw | | | | | | | | | | | | | | |
| | RW: | GH, | GM, | KE, | LS, | MW | MZ, | SD, | SL, | SZ | , TZ | ΰĠ, | ZW, | AT, | BE | , CH, | CY, |
| | | DE, | DK, | ES, | FI, | FR | GB, | GR, | ΙE, | ΙΊ | , LU | MC, | NL, | PT, | SE | , TR, | BF, |
| | | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GW, | ML | , MR | NE, | SN, | TD, | TG | | |
| ÇA | 2396 | 579 | | | A1 | | 2001 | 0705 | | CA | 2000- | 2396 | 579 | | | 20001 | 229 |
| EP | 1242 | 382 | | | A1 | | 2002 | 0925 | | ΕP | 2000- | 9884 | 37 | | | 20001 | 229 |
| EP | 1242 | 382 | | | B1 | | 2007 | 0207 | | | | | | | | | |
| | R: | AT, | BE, | CH, | DE, | DK. | ES, | FR, | GB, | GR | ?, IT, | LI, | LU, | NL, | SE | , MC, | PT, |
| | | ΙE, | SI, | LT, | LV, | FI, | RO, | MK, | CY, | ΑI | , TR | | | | | | |
| BR | 2000 | 0168 | 78 | | Α | | | | | | 2000 | | | | | | |
| | 2003 | | | | | | | | | | 2001 | | | | | 20001 | 229 |
| CN | 1437 | 584 | | | A | | 2003 | 0820 | | CN | 2000- | 8192 | 09 | | | 20001 | 229 |
| CN | 1704 | 404 | | | Α | | 2005 | 1207 | | CN | 2005 | 1008 | 2252 | | | 20001 | 229 |
| AΤ | 3533 | 20 | | | T | | 2007 | | | | 2000- | | | | | 20001 | 229 |
| ES | 2281 | 372 | | | Т3 | | 2007 | 1001 | | ES | 2000 | -9884 | 37 | | | 20001 | 229 |
| MX | 2002 | PA06 | 086 | | Α | | 2004 | 0823 | | | 2002 | | | | | 20020 | |
| RIORIT | Y APP | LN. | INFO | . : | | | | | | US | 1999 | 4736 | 00 | | A | 19991 | 229 |
| | | | | | | | | | | CN | 2000- | 8192 | 09 | | A 3 | 20001 | 229 |
| | | | | | | | | | | WO | 2000- | ·US35 | 616 | 1 | W | 20001 | 229 |
| THER S | OURCE | (S): | | | MAR | PAT | 135: | 92639 | 9 | | | | | | | | |

II

Page 20

GI

IT

The title compds. I [Ar = (un) substituted cycloalkyl, pyridyl, AΒ pyrimidinyl, etc.; n = 0-1; X = NH, O, S, NR; R = alkyl; Y, Z = both carbon or N; A = (un) substituted benzo, pyrido, pyrimido, etc.] which are useful as inhibitors of protein tyrosine kinase and are antiproliferative agents, were prepared E.g., a 3-step synthesis of II which showed IC50 of 0.005 µM against EGF-R kinase (recombinant enzyme), was given. 348618-70-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted aromatic tricyclic compds. containing nicotinonitrile

rings as protein kinase inhibitors)

348618-70-2 CA RN

3-Quinolinecarboxylic acid, 2-amino-6,7-dimethoxy-, methyl ester (CA CN INDEX NAME)

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

132:279125 CA

TITLE:

Synthesis of 1,2,3,4-tetrahydrodibenzo[b,g][1,8]naphth

yridines

AUTHOR(S):

Prakash, G. Arul; Rajendran, S. P.

CORPORATE SOURCE:

Department of Chemistry, Bharathiar University,

Coimbatore, 641 046, India

SOURCE:

Heterocyclic Communications (2000), 6(1), 63-66

CODEN: HCOMEX; ISSN: 0793-0283

PUBLISHER:

Freund Publishing House Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB 2-Chloro-3-formylquinoline and its derivs. were prepared and aminated by dry ammonia gas in ethanol. The 2-amino-3-formylquinolines so obtained were then condensed with cyclohexanone in presence of acetic acid and sulfuric acid to give 1,2,3,4-tetrahydrodibenzo[b,g][1,8]naphthyridines.

IT 264135-40-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tetrahydrodibenzonaphthyridines)

RN 264135-40-2 CA

CN 3-Quinolinecarboxaldehyde, 2-amino-7-methoxy- (CA INDEX NAME)

MeO NH2

REFERENCE COUNT:

7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

125:300981 CA

TITLE:

Preparation of 5,10-dihydropyrimido[4,5-b]quinolin-

4(1H)-ones as tyrosine kinase inhibitors

INVENTOR(S): PATENT ASSIGNEE(S): Dow, Robert L. Pfizer Inc., USA

SOURCE:

PCT Int. Appl., 22 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

GI

English

1

Ι

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|--------------|-------------------|----------------|
| | | | | |
| WO 9628444 | A1 | 19960919 | WO 1995-IB172 | 19950315 |
| W: CA, FI, JP, | MX, US | • | | |
| RW: AT, BE, CH, | DE, DK | , ES, FR, GB | , GR, IE, IT, LU, | MC, NL, PT, SE |
| US 5908930 | A | 19990601 | US 1997-894587 | 19970822 |
| PRIORITY APPLN. INFO.: | | | WO 1995-IB172 | W 19950315 |
| OTHER SOURCE(S): | MARPAT | 125:300981 | | |

Title compds. [I; R1 = H, (un) substituted alkyl; R2 = H, alkyl, AB alkoxycarbonyl, etc.; R3,R4 = H, (halo)alkyl, alkoxy, etc.] were prepared tyrosine kinase inhibitors (no data). Thus, 7,8-dimethoxy-4-oxo-3,4,5,10-tetrahydropyrimido[4,5-b]quinoline was treated with (MeO)2SO2/NaOH to give 5,10-dihydro-7,8-dimethoxy-3-methylpyrimido[4,5-b]quinolin-4(1H)-one.

IT 55149-43-4P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 5,10-dihydropyrimido[4,5-b]quinolin-4(1H)-ones as tyrosine kinase inhibitors)

RN 55149-43-4 CA

CN 3-Quinolinecarboxamide, 2-amino-6,7-dimethoxy- (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \end{array} \begin{array}{c} \text{NH}_2 \\ \text{C-NH}_2 \\ \text{O} \end{array}$$

L4 ANSWER 14 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

121:83189 CA

TITLE:

Synthesis and antimicrobial evaluation of novel quinoline-3-carboxylic acids and triazolo[4,3-

a]quinoline-4-carboxylic acids

AUTHOR(S):

El-Sayed, Ola A.; El-Semary, Mona A.; Khalil, Mounir

Α.

CORPORATE SOURCE:

Fac. Pharm., Univ. Alexandria, Alexandria, Egypt

SOURCE:

Alexandria Journal of Pharmaceutical Sciences (1993),

7(2), 163-6

CODEN: AJPSES; ISSN: 1110-1792

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB 2-Hydrazino-3-quinolinecarboxylic acids (I; R = H, Me, MeO), prepared from 2-chloro-3-quinolinecarboxaldehydes, were converted to triazoloquinolinecarboxylic acids such as II (same R). Several products showed modest bactericidal activity, but none showed fungicidal activity.

IT 155983-23-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactions of)

RN 155983-23-6 CA

CN 3-Quinolinecarboxylic acid, 2-hydrazino-7-methoxy- (9CI) (CA INDEX NAME)

CA COPYRIGHT 2007 ACS on STN ANSWER 15 OF 23

ACCESSION NUMBER:

114:185400 CA

TITLE:

Synthesis of some fused quinoline derivatives

Shehata, Ihsan A. AUTHOR(S):

CORPORATE SOURCE: SOURCE:

Fac. Pharm., Univ. Mansoura, Mansoura, Egypt Monatshefte fuer Chemie (1990), 121(12), 1017-21

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 114:185400

GI

- N

The furo[2,3-b] quinoline I was prepared from 6,7-dimethoxyquinoline 1-oxide AB in several steps, while the s-triazolo[4,3-a]quinoline II and tetrazolo[1,5-a]quinoline III were prepared from 6,7-dimethoxy-3-carboxyquinoline 1-oxide (IV) in several steps. Thus, chlorination of IV followed by condensation with hydrazine and cyclocondensation with sodium nitrite gave III.

III

IT 133406-54-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation of, with formaldehyde, triazoloquinoline from)

RN133406-54-9 CA

3-Quinolinecarboxylic acid, 2-hydrazino-6,7-dimethoxy- (9CI) CN NAME)

ANSWER 16 OF 23 CA COPYRIGHT 2007 ACS on STN

93:204581 CA ACCESSION NUMBER: ORIGINAL REFERENCE NO.:

93:32645a,32648a

TITLE: A facile base catalyzed condensation for the synthesis

of fused pyrimidine-2-carboxylic acid esters

Nakanishi, Susumu; Massett, Stephen S. AUTHOR(S):

Cent. Res., Pfizer Inc., Groton, CT, 06340, USA CORPORATE SOURCE: Organic Preparations and Procedures International SOURCE:

(1980), 12(3-4), 219-23

CODEN: OPPIAK; ISSN: 0030-4948

DOCUMENT TYPE:

Journal English LANGUAGE:

CASREACT 93:204581 OTHER SOURCE(S):

GI

The ester I (X = CH) was obtained in 99% yield by condensing AB 2-H2NC6H4CONH2 with (EtO2C)2 in the presence of NaOEt at 20-5°. I (X = N) was similarly obtained in 90% yield and II (R = R1 = H, OMe; R =Cl, R1 = H) were obtained in 92-9.5% yield. The reaction times were 15 min-48 h at 20-5°.

55149-43-4

RL: RCT (Reactant); RACT (Reactant or reagent) (cyclocondensation of, with oxalate in presence of sodium ethoxide)

55149-43-4 CA RN

3-Quinolinecarboxamide, 2-amino-6,7-dimethoxy- (CA INDEX NAME) CN

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \\ \text{NH}_2 \\ \\ \text{C-NH}_2 \\ \\ \\ \text{O} \end{array}$$

L4 ANSWER 17 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: ORIGINAL REFERENCE NO.:

92:121570 CA 92:19668h,19669a

TITLE:

Structure-activity relationships in a series of novel 3,4-dihydro-4-oxopyrimido[4,5-b]quinoline-2-carboxylic

acid antiallergy agents

AUTHOR (S):

Althuis, T. H.; Kadin, S. B.; Czuba, L. J.; Moore, P.

F.; Hess, H. J.

CORPORATE SOURCE:

SOURCE:

Cent. Res., Pfizer, Inc., Groton, CT, 06340, USA Journal of Medicinal Chemistry (1980), 23(3), 262-9

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE:

LANGUAGE:

Journal English

I

GI

The title compds. I [R = H, Me, CO2Et, CO2H, CONH2, etc., R1 = H, Me, AB CH2CO2Et, or (CH2)3 CO2Et; R2 = H or Ph; R3 = H, C1, or MeO; R4 and R5 = HH, F, MeO, etc; R6 = H or MeO] were prepared by condensation of the appropriate aminoquinolinecarboxamide (intermediate) with dialkyl oxalates or alkyl oxamates. The intermediates were prepared by base-catalyzed condensation of o-aminobenzaldehydes with 2-cyanoacetamide [107-91-5] or Knoevenagel condensation of o-nitroaldehydes with cyanoacetamide. The ability of I to interfere with the passive cutaneous anaphylaxis reaction was measured in male rats. Some I had i.v. potencies 100-400 times that of disodium cromoglycate (DSCG), and unlike DSCG which is inactive orally, some I possessed oral activity. Et 7-ethoxy-3,4-dihydro-8-methoxy-4oxopyrimido[4,5-b]quinoline-2-carboxylate [55149-13-8] and Et 3,4-dihydro-7-hydroxy-8-methoxy-4-oxopyrimido[4,5-b]quinoline-2carboxylate trifluoroacetate salt [58662-62-7] were the most effective. A CO2H in position 2 afforded optimal activity and esters showed good oral absorption. Structure-activity relations are discussed.

IT 55149-43-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with dialkyloxylates and alkyloxymates)

RN 55149-43-4 CA

CN 3-Quinolinecarboxamide, 2-amino-6,7-dimethoxy- (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{N} & \text{NH}_2 \\ \\ \text{MeO} & & \text{C-NH}_2 \\ \\ \text{O} & & \\ \end{array}$$

ANSWER 18 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: ORIGINAL REFERENCE NO.:

87:168090 CA 87:26571a,26574a

TITLE:

Fused pyrimidin-4(3H)-ones as antiallergy agents Althuis, Thomas H.; Czuba, Leonard J.; Hess, Hans

Jurgen E.; Kadin, Saul B.

PATENT ASSIGNEE(S):

Pfizer Inc., USA

SOURCE:

U.S., 31 pp. Division of U.S. 3,974,161.

CODEN: USXXAM

DOCUMENT TYPE:

INVENTOR(S):

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|------------------------|-------|----------|-----------------|------------|----------|
| US 4044134 | А | 19770823 | US 1976-667515 | | 19760316 |
| SE 7404011 | Α | 19741014 | SE 1974-4011 | | 19740325 |
| SE 401185 | C | 19780803 | | | |
| SE 401185 | В | 19780424 | | | |
| US 3974161 | A | 19760810 | US 1974-485945 | | 19740705 |
| GB 1501438 | Α | 19780215 | GB 1975-18583 | | 19750502 |
| IL 47233 | ·A | 19800131 | IL 1975-47233 | | 19750505 |
| AT 7607580 | Α | 19770715 | AT 1976-7580 | | 19761012 |
| AT 7607579 | Α | 19771115 | AT 1976-7579 | | 19761012 |
| US 4120962 | Α | 19781017 | US 1977-786185 | | 19770411 |
| DK 7703873 | Α | 19770831 | DK 1977-3873 | | 19770831 |
| US 4134981 | Α | 19790116 | US 1977-845816 | | 19771027 |
| PRIORITY APPLN. INFO.: | | | US 1973-351025 | A2 | 19730413 |
| | | | US 1974-444138 | A2 | 19740220 |
| | | | US 1974-485945 | A3 | 19740705 |
| | | | GB 1973-55900 | Α | 19731203 |
| | | | IL 1974-44569 | Α | 19740404 |
| | | | DK 1974-2009 | Α | 19740410 |
| | | | AT 1974-3151 | Α | 19740416 |
| | | | US 1976-667515 | A 3 | 19760316 |
| | | | US 1977-786185 | A3 | 19770411 |

OTHER SOURCE(S):

MARPAT 87:168090

GI

Pyrimidoquinolonecarboxylates I (R = CO2Et, CO2H, CONH2, CONHOH, Me, Et, Ac, CO2Bu; R1 = H, OMe, OEt, SMe, SOMe, C1, F, OH, OAc; R2 = H, OMe, OEt, OBu, OC7H7; R3 = H, OMe), benzoquinazolenecarboxylates II (R4 = Et, H), pyridopyrimidinonecarboxylate III etc. were prepared Thus, 2-H2NC6H4CHO was condensed with NCCH2CONH2, and 2-amino-3-quinolinecarboxamide condensed with di-Et oxalate to give I (R = CO2Et, R1-R3 = H), which upon administration 1 mg/kg i.v. to rats gave 100% inhibition of passive cutaneous anaphylaxis.

IT 55149-43-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and condensation of, with diethyl oxalate)

RN 55149-43-4 CA

CN 3-Quinolinecarboxamide, 2-amino-6,7-dimethoxy- (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} & \text{N} & \text{NH}_2 \\ \\ \text{MeO} & \\ \\ \text{C} & \text{NH}_2 \\ \\ \\ \text{O} \end{array}$$

ANSWER 19 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 87:117902 CA ORIGINAL REFERENCE NO.: 87:18725a,18728a

TITLE:

2-Carboxypyrimido[4,5-b]quinolin-4(3H)-one esters

PATENT ASSIGNEE(S): Pfizer Inc., USA Neth. Appl., 12 pp. SOURCE:

CODEN: NAXXAN

DOCUMENT TYPE:

Patent

LANGUAGE:

Dutch

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------------|----------|------------------|----------|
| | | 10761006 | NT 1076 2002 | 10760220 |
| NL 7603293 | A | 19761026 | NL 1976-3293 | 19760330 |
| NL 161155 | C | 19800115 | | |
| NL 161155 | В | 19790815 | | |
| SE 7603133 | Α | 19761025 | SE 1976-3133 | 19760309 |
| CA 1065863 | A1 | 19791106 | CA 1976-247583 | 19760310 |
| DK 7601438 | Α | 19761025 | DK 1976-1438 | 19760330 |
| DK 142323 | В | 19801013 | | |
| DK 142323 | С | 19810629 | | |
| ES 446498 | A1 | 19770616 | ES 1976-446498 | 19760330 |
| SU 638261 | A3 | 19781215 | SU 1976-2343061 | 19760407 |
| CH 609056 | A5 | 19790215 | CH 1976-4398 | 19760407 |
| JP 51127098 | \mathbf{A} | 19761105 | JP 1976-41749 | 19760413 |
| JP 54003880 | В | 19790227 | | |
| AT 351549 | В | 19790725 | AT 1976-2700 | 19760413 |
| AT 7602700 | Α | 19790115 | | |
| FI 7601020 | Α | 19761025 | FI 1976-1020 | 19760414 |
| DD 125208 | A5 | 19770406 | DD 1976-192403 | 19760415 |
| PL 101824 | B1 | 19790228 | PL 1976-188875 | 19760417 |
| RO 68966 | A1 | 19810530 | RO 1976-85654 | 19760417 |
| PRIORITY APPLN. INFO.: | | | US 1975-571318 A | 19750424 |
| GI | | | | |

The antiallergic (no data) pyrimidoquinolinone I was prepared in 98.8% yield AB by condensing 2-amino-6,7-dimethoxy-3-quinolinecarboxamide with di-Et oxalate.

IT 55149-43-4

RL: RCT (Reactant); RACT (Reactant or reagent) (condensation of, with oxalate)

RN 55149-43-4 CA

3-Quinolinecarboxamide, 2-amino-6,7-dimethoxy- (CA INDEX NAME) CN

L4 ANSWER 20 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 87:85036 CA ORIGINAL REFERENCE NO.: 87:13535a,13538a

TITLE: Fused pyrimidine derivatives and preparation thereof

PATENT ASSIGNEE(S): Pfizer Inc., USA

SOURCE: Brit., 9 pp. Addn. to Brit. 1,458,205. CODEN: BRXXAA

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|------------------|----------|
| | | | | |
| GB 1465353 | Α | 19770223 | GB 1974-15536 | 19740408 |
| PRIORITY APPLN. INFO.: | | | US 1974-444138 A | 19740220 |

AB Nine pyrimidoquinolines I [R = HO(CH2)202C, Et02C, Et, Ac; R1 = H, Me, Et02CCH2, Et02C(CH2)3, AcO(CH2)2; R2 = MeO, MeS, MeSO; R3 = MeO, H] and the pyridopyrimidone II, useful as inhibitors of allergic reactions, especially of allergic bronchial asthma, were prepared I were prepared from Et 7,8-dimethoxy-4-oxo-(3H)-pyrimido[4,5-b]quinoline-2-carboxylate by standard methods or from the quinolines III by cyclocondensation reactions. II was prepared from 2-aminonicotinamide by stirring with concentrated H2SO4 and (EtCO)20

1 h at 60° followed by treatment with dilute alkali and reacidification. The antiallergy activities of some I on i.v. and oral administration to animals are reported.

IT 55149-43-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with propionic anhydride)

RN 55149-43-4 CA

CN 3-Ouinolinecarboxamide, 2-amino-6,7-dimethoxy- (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{N} & \text{NH}_2 \\ \\ \text{MeO} & & \text{C-NH}_2 \\ \\ \text{O} & & \\ \end{array}$$

ANSWER 21 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: ORIGINAL REFERENCE NO.: 84:19797a,19800a

84:121894 CA

TITLE:

Condensed pyridine-4-(3H)-ones

INVENTOR(S):

Althuis, Thomas H.; Czuba, Leonard J.; Hess, Hans J.

E.; Kadin, Saul B.

PATENT ASSIGNEE(S):

Pfizer Inc., USA

SOURCE:

Ger. Offen., 70 pp. Addn. to Ger. Offen. 2,418,498.

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|----------------------|------------|----------|-----------------|-------------|
| • | DE 2525050 | A1 | 19760122 | DE 1975-2525050 | 19750603 |
| | US 3974161 | A | 19760810 | US 1974-485945 | 19740705 |
| | CA 1053674 | A1 | 19790501 | CA 1975-225936 | 19750430 |
| | GB 1501438 | A | 19780215 | GB 1975-18583 | 19750502 |
| | NO 7501594 | A | 19760106 | NO 1975-1594 | 19750505 |
| | IL 47233 | Α | 19800131 | IL 1975-47233 | 19750505 |
| | ZA 7502908 | A | 19760428 | ZA 1975-2908 | 19750506 |
| | AU 7580955 | Α | 19761111 | AU 1975-80955 | 19750508 |
| | ES 437966 | A2 | 19770216 | ES 1975-437966 | 19750527 |
| | FI 7501628 | A | 19760106 | FI 1975-1628 | 19750603 |
| | FI 59097 | В | 19810227 | | |
| | FI 59097 | C | 19810610 | | |
| | DK 7502502 | A | 19760106 | DK 1975-2502 | 19750604 |
| | RO 69550 | A1 | 19810830 | RO 1975-82428 | 19750604 |
| | NL 7506665 | Α | 19760107 | NL 1975-6665 | 19750605 |
| | NL 173270 | В | 19830801 | | |
| | NL 173270 | C | 19840102 | | |
| | BE 829987 | A4 | 19751208 | BE 1975-1006719 | |
| | JP 51008280 | A | 19760123 | JP 1975-68456 | 19750606 |
| | FR 2276825 | A2 | 19760130 | FR 1975-17789 | 19750606 |
| | FR 2276825 | B2 | 19781110 | | |
| | AT 351546 | В | 19790725 | AT 1975-4326 | 19750606 |
| | AT 7504326 | Α | 19790115 | | |
| | CH 619951 | A 5 | 19801031 | CH 1975-7300 | 19750606 |
| | SE 7504599 | Α | 19760107 | SE 1975-4599 | 19750621 |
| | SE 420610 | C | 19820128 | | |
| PR | IORITY APPLN. INFO.: | | | US 1974-485945 | A 19740705 |
| | | | | US 1973-351025 | A2 19730413 |
| | | | | GB 1973-55900 | A 19731203 |
| | | | • | US 1974-444138 | A2 19740220 |
| | | | | IL 1974-44569 | A 19740404 |
| | | | | | |

GI

$$R^1$$
 NH
 R^2
 $N = 1$
 $N =$

Pyrimidoquinolinones I (R = CO2Et, CO2Bu, CO2H, Me, Ac; R1 = OCH2Ph, OEt, OMe, OH, OAc; R2 = H, OMe, OEt, OCH2Ph, OH) (16 compds.) were prepared II (R3 = CHO) was treated with NCCH2CONH2, II [R3 = CH:C(CN)CONH2] reduced, III condensed EtO2CCO2Et, and I (R = CO2Et, R1 = OCH2Ph, R2 = OMe) debenzylated. I (R = CO2Et, R1 = OH, R2 = OMe) thus obtained at 0.0003 mg/kg i.v. gave 38% inhibition in passive cutaneous anaphylaxis test.

IT 55149-57-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and condensation of, with oxalate)

RN 55149-57-0 CA

CN 3-Quinolinecarboxamide, 2-amino-6-ethoxy-7-(phenylmethoxy)- (CA INDEX NAME)

ANSWER 22 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 82:73015 CA ORIGINAL REFERENCE NO.: 82:11675a,11678a TITLE: Molten pyrimidines

INVENTOR(S): Althuis, Thomas H.; Czuba, Leonard J.; Hess, Hans J.

E.; Kadin, Saul B.

PATENT ASSIGNEE(S): Pfizer, Chas., and Co., Inc.

Ger. Offen., 62 pp. SOURCE:

CODEN: GWXXBX

DOCUMENT TYPE: Patent.

German LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---------------------|------|----------|-----------------|---|----------|
| DE 2418498 | | 19741107 | DE 1974-2418498 | - | 19740411 |
| GB 1458205 | Α | 19761208 | GB 1973-55900 | | 19731203 |
| AU 7467500 | Α | 19751009 | AU 1974-67500 | | 19740403 |
| NO 139735 | С | 19790502 | NO 1974-1231 | | 19740404 |
| NO 139735 | В | 19790122 | | | |
| IL 44569 | Α | 19790531 | IL 1974-44569 | | 19740404 |
| NL 7404894 | A | 19741015 | NL 1974-4894 | | 19740410 |
| NL 170285 | В | 19820517 | | | |
| NL 170285 | C | 19821018 | • | | |
| ES 425238 | A1 | 19760516 | ES 1974-425238 | | 19740410 |
| FI 55658 | C | 19790910 | FI 1974-1095 | | 19740410 |
| FI 55658 | В | 19790531 | | | |
| DK 142621 | В | 19801201 | DK 1974-2009 | | 19740410 |
| DK 142621 | С | 19810803 | | | |
| BE 813571 | A1 | 19741011 | BE 1974-1005874 | | 19740411 |
| DD 111207 | A5 | 19750205 | DD 1974-177859 | | 19740411 |
| ZA 7402351 | A | 19750430 | ZA 1974-2351 | | 19740411 |
| CH 619950 | A5 | 19801031 | CH 1974-5110 | | 19740411 |
| FR 2225166 | Al | 19741108 | FR 1974-13092 | | 19740412 |
| JP 50018481 | A | 19750226 | JP 1974-41582 | | 19740413 |
| RO 64918 | A2 | 19790815 | RO 1974-78412 | | 19740413 |
| RO 64918 | A1 | 19800115 | | | |
| AT 7403151 | A | 19770815 | AT 1974-3151 | | 19740416 |
| GB 1501438 | A | 19780215 | GB 1975-18583 | | 19750502 |
| AT 7607580 | A | 19770715 | ÀT 1976-7580 | | 19761012 |
| AT 7607579 | Α | 19771115 | AT 1976-7579 | | 19761012 |
| DK 7703873 | Α | 19770831 | DK 1977-3873 | | 19770831 |
| ORITY APPLN. INFO.: | | | US 1973-351025 | Α | 19730413 |
| | | | GB 1973-55900 | Α | 19731203 |
| | | | DK 1974-2009 | A | 19740410 |
| | | | AT 1974-3151 | A | 19740416 |
| | | | US 1974-485945 | Α | 19740705 |

GI For diagram(s), see printed CA Issue. Twenty-seven pyrimidoquinolines I [R = Me, Et, Ac, CO2R7 (R7 = H, Na, Et, Bu, CH2CH2OH), CONH2, CONHOH; R1 = H, Ph; R2 = H, C1, MeO; R3 = H, MeO, F,AB Cl, EtO, MeS, MeS(O); R4 = H, MeO, EtO, BuO, PhCH2O, F; R3R4 = OCH2O, OCH2CH2O; R5 = H, MeO; R6 = Me, CH2CO2Me, (CH2)3CO2Et, (CH2)2OAc], Et benzo[g]quinazolin-4(3H)-one-2-carboxylate, Et pyrido[2,3-d]pyrimidin-4(3H)-one-2-carboxylate, and 2-ethylpyrimido[2,3-d]pyrimidin-4(3H)-one, useful as inhibitors of bronchial asthma, were prepared: a) by condensation of cyanoacetamide with a nitrobenzaldehyde to give acrylamide II which was cyclized with powdered Fe in AcOH or AcOH-DMF to aminoquino-linecarboxamide III. Refluxing III with an oxalate ester and aromatic hydrocarbon gave I. b) Cyanoacetamide condensed with an aminobenzaldehyde gave III directly.

Many of the compds. prepared had 100% antiallergic activity at 1-10 mg/kg (average of 8 animals) i.v.

IT 55149-43-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and cyclization with diethyl oxalate)

RN 55149-43-4 CA

CN 3-Quinolinecarboxamide, 2-amino-6,7-dimethoxy- (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{N} & \text{NH}_2 \\ \\ \text{MeO} & \text{C-NH}_2 \\ \\ \text{O} \end{array}$$

ANSWER 23 OF 23 CA COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 50:16402 CA

50:3443h-i,3444a-h ORIGINAL REFERENCE NO.:

TITLE: Synthesis of fused heterocyclics AUTHOR (S): Somasekhara, I. S.; Phadke, Ragini

Indian Inst. Sci., Bangalore CORPORATE SOURCE:

Journal of the Indian Institute of Science (1955), SOURCE:

37A, 120-9

CODEN: JIISAD; ISSN: 0019-4964

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

Dihydronaphthinoline (I) was prepared by refluxing 150 mg. AB tetrahydronaphthinoline (II) [Reissert, Ber. 27, 2244(1894)] and 360 mg. chloranil in 30 ml. xylene for 4 hrs. The red precipitate dissolved in Et20

was

extracted 3 times with 10% NaOH to remove tetrachlorohydroquinone, dried over anhydrous Na2SO4, passed through a column of alumina, gave 2 bands under ultraviolet light. The first gave 30 mg. II and the second gave 70 mg. I, m. 200° (from EtOH). I was also obtained in 70 mg. yield by heating a mixture of 100 mg. II and 400 mg. Se at 280-300° for 15 hrs. The solid, treated as above, gave the identical product. 4'-Hydroxyquinolino(2,3,2',3')quinoline (III) was obtained, when 250 mg. II, aqueous Na2Cr2O7 (1.2 g. in 50 ml. H2O), and 2 ml. concentrated H2SO4 were refluxed for 8 hrs. The precipitate, in 100 ml. H2O, made alkaline with 20

ml. aqueous

AcOH,

NH3, neutralized with AcOH and extracted with CHCl3, yielded a yellow solid, bright yellow needles on sublimation, m. 280° (with charring), soluble in AcOH, alc. solution bright yellow with green fluorescence, red on addition of alkali. Di-Et (6-nitroveratrylidene) malonate (IV) was obtained in 10 g. yield when a mixture of 10 g. 6-nitroveratraldehyde (V), 1.8 moles CH2(CO2Et)2, 6 ml. piperidine, and 8 ml. pyridine after 7 days at room temperature, added to 50 g. ice containing 10 ml. concentrated HCl; gummy mass recrystd.

from EtOH gave yellow needles, m. 118-20°, soluble in Me2CO, EtOH, and AcOEt. IV, dissolved in 50 ml. cold EtOH and 20 ml. aqueous NH2, H2S added for 5 hrs. (40 ml. NH3 added during the reaction), the solid washed with H2O and EtOH, dried, yielded 0.3 g. Et 6,7-dimethoxy-2-hydroxyquinoline-3-carboxylate (VI), m. 270-71°, alc. solution gave blue fluorescence. VI, saponified with 10% aqueous KOH for 2 hrs., filtered and acidified with

cooled, gave 6,7-dimethoxy-2-hydroxyquinoline-3-carboxylic acid (VII), m. 320° (decompose) (from AcOH), blue fluorescence in EtOH. VII sublimed twice at 7 mm. and 400° for 20 min. gave a sublimate, m. 235°; fractionally crystallized from EtOH, the less soluble VII crystallized first, and 6,7-dimethoxy-2-hydroxyquinoline (VIII), m. 230°, from the mother liquor. VI (0.7 g.) refluxed with 5 ml. POCl3 for 30 min., excess POC13 removed under reduced pressure, the solid residue heated with 1.5 ml. distilled PhNH2 at 140° for 2 hrs. yielded 0.6 g. 6,7-dimethoxy-2-hydroxyquinoline-3-carboxylic acid anilide (IX), yellow needles, m. 360-51° (from AcOH), stable to alkaline hydrolysis, alc. solution gave blue fluorescence on addition of alkali. Et 6,7-dimethoxy-2-anilinoquinoline-3-carboxylate (X) was obtained in 0.5 q. yield by heating 0.5 g. VI and 1 ml. POCl $\bar{3}$ heated at 100° for 30 min., excess POCl3 removed, 0.5 ml. PhNH2 added and again heated at 100° for 30 min.; the solid, taken up in 5 ml. hot AcOH, cooled, neutralized with NH3, gave a yellow solid, m.p. 167° (from dilute AcOH). X saponified with alc. KOH (5%) for 3 hrs. gave after distilling off EtOH, 0.4 g. 6,7-dimethoxy-2-anilinoquinoline-3-carboxylic acid (XI), m.

244-45° (from dilute AcOH). X (0.2 g.) treated with POCl3 (1.5 ml.) at 100° for 30 min., cooled, 10 ml. H2O added, refluxed, yielded

0.10 g. 4'-hydroxy-6,7-dimethoxyquinolino(2,3,2',3')quinoline (XII), m.
290° (from dilute AcOH), alc. solution deep yellow with green
fluorescence changing to red on addition of alkali. V (6 g.), CH2(CO2H)2
(6 g.), piperidine (2 ml.), and pyridine (10 ml.) heated at 100°
for 4 hrs., treated with cold dilute HCl gave 4.6 g. 6-nitro-3,4dimethoxycinnamic acid (XIII), m. 285° (from AcOH). XIII (4.6 g.)
in 350 ml. absolute EtOH and 15 ml. concentrated H2SO4 refluxed for 4 hrs.,
the EtOH

distilled off, the residue washed with dilute NH3, gave Et 6-nitro-3,4-dimethoxycinnamate (XIV), m. 148° (from EtOH). XIV (1 g.) in EtOH-AcOEt mixture (10:15), aqueous FeSO4 (10 g. in 30 ml. H2O) and 20 ml. liquid NH3 added, refluxed for 30 min. on water bath, filtered, the filtrate diluted and extracted with AcOEt, the extract dried over MgSO4, AcOEt removed, gave 0.3 g. Et 6-amino-3,4-dimethoxycinnamate (XV), m. 92° (from Et2O-petr. ether). 6,7-Dimethoxy-2-hydroxyquinoline (XVI) was prepared through 3 different procedures: (a) 0.1 g. XV dissolved in 10 ml. boiling concentrated HCl, the acid evaporated off on a water bath,

residue treated with aqueous NH4OAc, gave a few mg. of XVI, m. 225°;
(b) XIV (1 g.) refluxed for 2 hrs. with 5 g. Zn dust and 100 ml. 5% AcOH, filtered hot, cooled, the filtrate extracted with Et2O, let stand overnight, gave 0.2 g. XVI, m. 229° (from Me2CO); (c) a trace yield according to Kefford (C.A. 34, 7918.1).

IT 860205-98-7P, 3-Quinolinecarboxylic acid, 2-anilino-6,7-dimethoxy, ethyl ester

RL: PREP (Preparation) (preparation of)

RN 860205-98-7 CA

CN 3-Quinolinecarboxylic acid, 2-anilino-6,7-dimethoxy-, ethyl ester (5CI) (CA INDEX NAME)

```
10/530986
```

=> d his

(FILE 'HOME' ENTERED AT 11:03:30 ON 18 DEC 2007)

FILE 'REGISTRY' ENTERED AT 11:03:38 ON 18 DEC 2007

L1 STRUCTURE UPLOADED

L2 13 S L1 SAM

L3 208 S L1 FULL

FILE 'CA' ENTERED AT 11:04:02 ON 18 DEC 2007

L4 23 S L3

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

STN INTERNATIONAL LOGOFF AT 11:04:46 ON 18 DEC 2007